A family of rules for parameter choice in Tikhonov regularization of ill-posed problems with inexact noise level

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Contents

- We consider linear ill-posed problems

$$Ax = y_*, \qquad y_* \in \mathcal{R}(A),$$

where $A\colon X \to Y$ is a linear continuous operator between Hilbert spaces. The range $\mathcal{R}(A)$ may be non-closed and the kernel $\mathcal{N}(A)$ may be non-trivial.

- Assume that instead of exact data y_* only its approximation y is available.
- For approximation of the minimum norm solution x_* of the problem $Ax = y_*$ we use the Tikhonov regularization method

$$x_\alpha = (\alpha I + A^* A)^{-1} A^* y.$$

Information about noise level

- In the following we consider three cases of knowledge about noise level for $\|y - y_*\|$:
  - Case 1: exact noise level δ: $\|y - y_*\| \leq \delta$.
  - Case 2: no information about $\|y - y_*\|$.
  - Case 3: approximate noise level: given is δ but it is not known whether the inequality $\|y - y_*\| \leq \delta$ holds or not. For example, it may be known that with high probability $\delta/\|y - y_*\| \in [1/10, 10]$. This very useful information should be used for choice of $\alpha = \alpha(\delta)$.
- Choice of regularization parameter α.
  - Rules for the Case 1 (discrepancy principle, etc.) need exact noise level: rules fail for very small underestimation of the noise level and give large error $\|x_\alpha - x_*\|$ already for 10% overestimation.
  - Rules for the Case 2 do not guarantee the convergence $x_\alpha \to x_*$ for $\|y - y_*\| \to 0$.
  - Our rules for the Case 3 guarantee $x_\alpha \to x_*$ as $\delta \to 0$, if $\lim_{\delta \to 0} \frac{\|y - y_*\|}{\delta} \leq \text{const}$.

Parameter choice rules for the case of exact noise level

- Discrepancy principle (D): α_{D} is the solution of $d_{\mathrm{D}}(\alpha) := \|Ax_\alpha - y\| = C\delta,\ C \geq 1$.
- Monotone error rule (ME):

$$d_{\mathrm{ME}}(\alpha) := \frac{\|B_\alpha(Ax_\alpha - y)\|^2}{\|B_\alpha^2(Ax_\alpha - y)\|} = \delta,$$

$$B_\alpha = \sqrt{\alpha}(\alpha I + AA^*)^{-1/2}.$$

Family of rules for parameter choice

Fix q, l, k such that $3/2 \le q < \infty$, $l \ge 0$, $k \ge l/q$; $2q$, $2k$, $2l \in \mathbb{N}$.
Choose $\alpha = \alpha(\delta)$ as the largest solution of

$$d(\alpha \mid q, l, k) := \frac{\kappa(\alpha) \| D_\alpha^k B_\alpha (Ax_\alpha - y)\|^{q/(q-1)}}{\| D_\alpha^l B_\alpha^{2q-2}(Ax_\alpha - y)\|^{1/(q-1)}} = b\delta,$$

where $B_\alpha = \sqrt{\alpha}(\alpha I + AA^*)^{-1/2}$, $D_\alpha = \alpha^{-1} AA^* B_\alpha^2$,

$$\kappa(\alpha) = \begin{cases} 1, & \text{if } k = l/q, \\ (1 + \alpha \|A\|^{-2})^{\frac{kq - l + q/2}{q-1}}, & \text{if } k > l/q, \end{cases} \tag{1}$$

$$\downarrow \ \alpha \to 0 \qquad\qquad 1 \tag{2}$$

$$b \approx \left(\frac{3}{2}\right)^{\frac{3}{2}} \frac{k^k}{(k+3/2)^{k+3/2}} \left(\frac{k^k (l+3/2)^{l+3/2}}{l^l (k+3/2)^{k+3/2}}\right)^{\frac{1}{q-1}}. \tag{3}$$

Denote this rule by R(q, l, k).

Examples of this family of rules

- Modified discrepancy principle (Raus 1985, Gfrerer 1987): $q = 3/2$, $l = k = 0$
- Monotone error rule (Tautenhahn 1998): $q = 2$, $l = k = 0$
- Rule R1 (Raus 1992): $q = 3/2$, $k = l > 0$
- Balancing principle (Mathé, Pereverzev 2003) can be considered as an approximate variant of rule R1 with $k = 1/2$.

Existence of solution for family of rules

1. If $k > l/q$, then the equation $d(\alpha \mid q, l, k) = b\delta$ has a solution for every $b = \text{const} > 0$, because $\lim_{\alpha\to\infty} d(\alpha \mid q, l, k) = \infty$ and $\lim_{\alpha\to 0} d(\alpha \mid q, l, k) = 0$.
2. If $k = l/q$, then the solution of the equation $d(\alpha \mid q, l, k) = b\delta$ exists, if $b \geq b_0(q, l, k)$ and $\|y - y_*\| \leq \delta$.

Convergence and stability

- **Convergence.** Let $k \geq l/q$. Let the parameter $\alpha = \alpha(\delta)$ be the solution of the equation $d(\alpha \mid q, l, k) = b\delta$, $b > b_0(q, l, k)$. If $\|y - y_*\| \leq \delta$, then $\|x_\alpha - x_*\| \to 0$ $(\delta \to 0)$.
- **Stability** (with respect to the inaccuracy of the noise level). Let $k > l/q$. Let the parameter $\alpha(\delta)$ be the **largest** solution of the equation $d(\alpha \mid q, l, k) = b\delta$. If $\frac{\|y-y_*\|}{\delta} \leq c = \text{const}$ in the process $\delta \to 0$, then $\|x_\alpha - x_*\| \to 0$ $(\delta \to 0)$.

Quasioptimality

Let $l/q \leq k \leq l \leq q/2$. Let the parameter $\alpha(\delta)$ be the **smallest** solution of the equation $d(\alpha \mid q, l, k) = b\delta$. Then the rule is ***quasioptimal***:

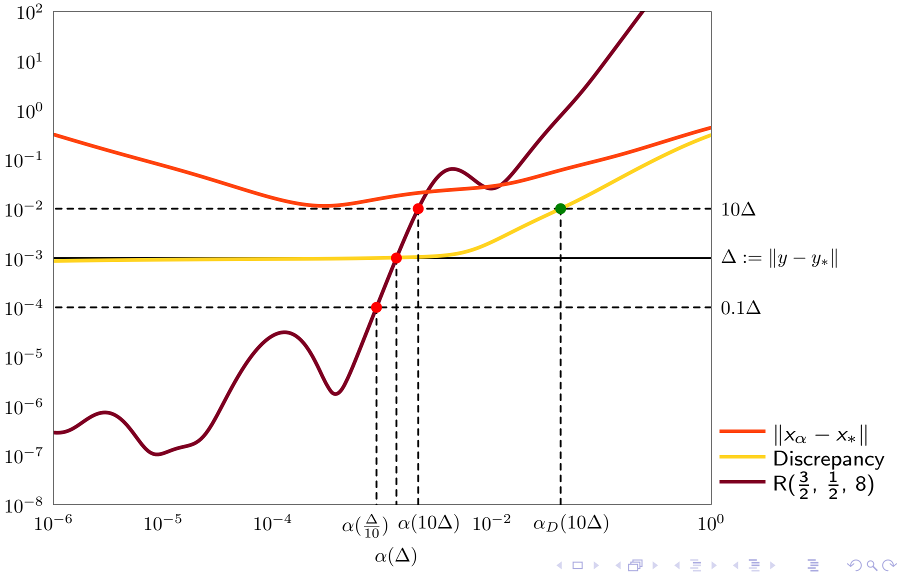
$$\|x_\alpha - x_*\| \leq C(b) \inf_{\alpha \geq 0} \left\{ \|x_\alpha^+ - x_*\| + \frac{\delta}{2\sqrt{\alpha}} \right\},$$

where x_α^+ is the approximate solution with exact right-hand side. It holds $\sup_{\|y-y_*\|\leq\delta} \|x_\alpha - x_\alpha^+\| \leq \frac{\delta}{2\sqrt{\alpha}}$

- Largest solution $\Rightarrow$ stability
- Smallest solution $\Rightarrow$ quasi-optimality
- If the solution is unique, quasi-optimality also holds for the largest solution. In most of our numerical experiments the solution was unique.

In the following we choose the largest solution.

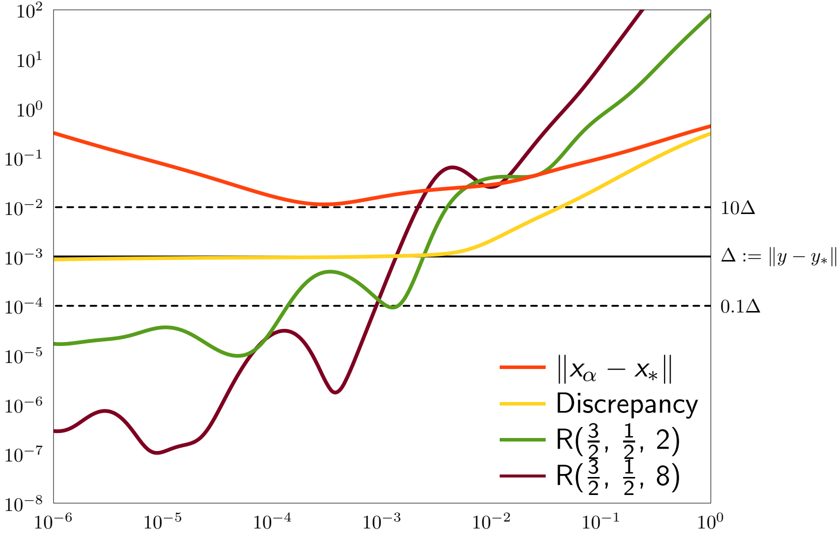
Stability of choice $\alpha = \alpha(\delta)$ from rule $d(\alpha) = \delta$



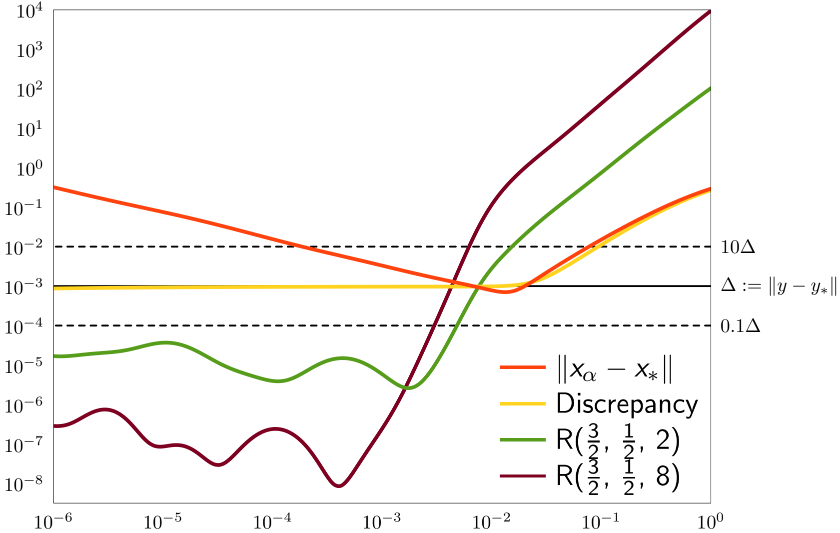
Stability of parameter choice

- Compare rules for choice of the regularization parameter $\alpha = \alpha(\delta)$ as the solution of the equation $d(\alpha) = b\delta$.
- The stability of parameter choice rule with respect to the inaccuracy of noise level information increases for increasing $d'(\alpha)$ in the neighbourhood of $\alpha(\|y - y_*\|)$.
- In many rules from the family $d'(\alpha)$ is much larger than in the discrepancy principle, thus these rules are more stable with respect to inaccuracies of noise level $\delta \approx \|y - y_*\|$.
- The previous slide and the following 3 slides show the behaviour of functions $d(\alpha)$ in the problem 'phillips' from Hansen's Regularization Tools.

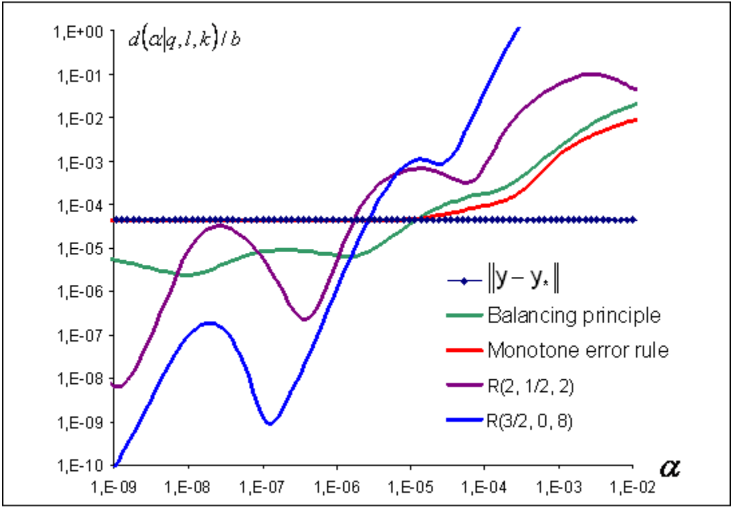
Behavior of functions $d(\alpha)$ in rules $d(\alpha) = \delta$, $p = 0$



Behavior of functions $d(\alpha)$ in rules $d(\alpha) = \delta$, $p = 2$



Behaviour of function $d(\alpha)$ in the neighbourhood $\alpha(\|y - y_*\|)$, $p = 0$



Hansen's test problems used in numerical tests.

Set I of test problems, P. C. Hansen's *Regularization Tools*.

Nr	Problem	cond_{100}	selfadj	Description
1	baart	5e+17	no	(Artificial) Fredholm integral equation of the first kind
2	deriv2	1e+4	yes	Computation of the second derivative
3	foxgood	1e+19	yes	A problem that does not satisfy the discrete Picard condition
4	gravity	3e+19	yes	A gravity surveying problem
5	heat	2e+38	no	Inverse heat equation
6	ilaplace	9e+32	no	Inverse Laplace transform
7	phillips	2e+6	yes	An example problem by Phillips
8	shaw	5e+18	yes	An image reconstruction problem
9	spikes	3e+19	no	Test problem whose solution is a pulse train of spikes
10	wing	1e+20	no	Fredholm integral equation with discontinuous solution

Brezinski-Rodriguez-Seatzu problems

Set II of test problems, *Numerical Algorithms* 2008, 49, 1–4, pp 85–104.

Nr	Problem	cond_{100}	selfadj	Description
11	gauss	6e+18	yes	Test problem with Gauss matrix $a_{ij} = \sqrt{\frac{\pi}{2\sigma}} e^{-\frac{\sigma}{2(i-j)^2}}$, kus $\sigma = 0.01$
12	hilbert	4e+19	yes	Test problem with Hilbert matrix $a_{ij} = \frac{1}{i+j-1}$
13	lotkin	2e+21	no	Test problem with Lotkin matrix (same as Hilbert matrix, except $a_{1j} = 1$)
14	moler	2e+4	yes	Test problem with Moler matrix $A = B^T B$, where $b_{ii} = 1$, $b_{i,i+1} = 1$, and $b_{ij} = 0$ otherwise
15	pascal	1e+60	yes	Test problem with Pascal matrix $a_{ij} = \binom{i+j-2}{i-1}$
16	prolate	1e+17	yes	Test problem with a symmetric, ill-conditioned Toeplitz matrix

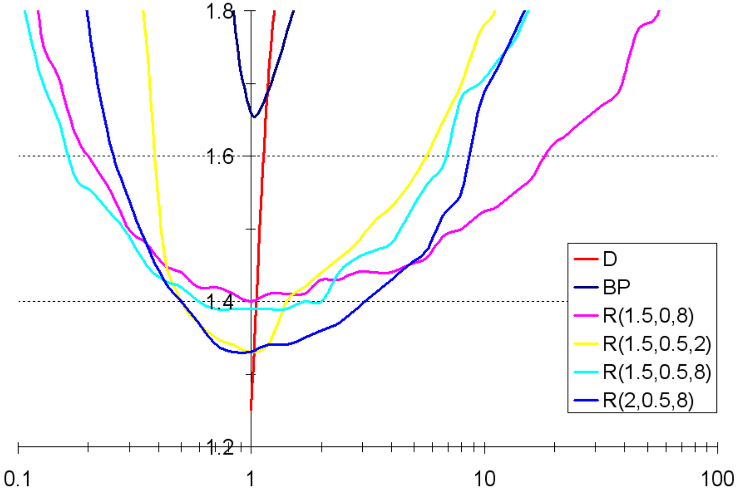
Solution vectors for BRS-problems

Description	$\overline{x}_i$
constant	1
linear	$\frac{i}{N}$
quadratic	$\left(\frac{i-\lfloor\frac{N}{2}\rfloor}{\lceil\frac{N}{2}\rceil}\right)^2$
sinusoidal	$\sin\frac{2\pi(i-1)}{N}$
linear+sinusoidal	$\frac{i}{N}+\frac{1}{4}\sin\frac{2\pi(i-1)}{N}$
step function	$\begin{cases}0, & \text{if } i\leq\lfloor\frac{N}{2}\rfloor\\ 1, & \text{if } i>\lfloor\frac{N}{2}\rfloor\end{cases}$

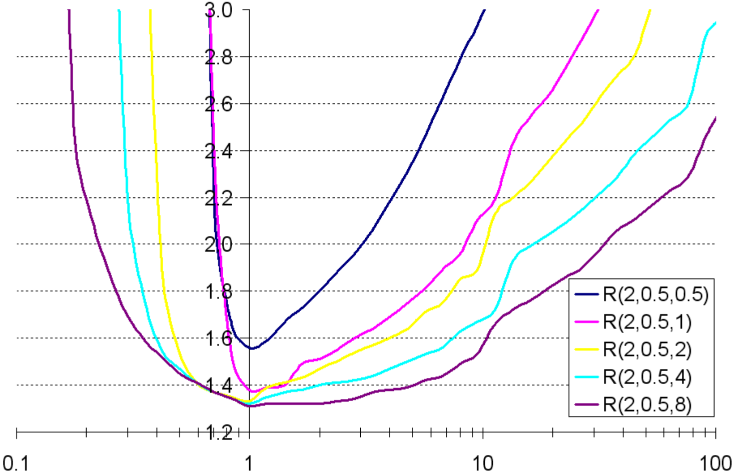
Perturbed data and presentation of results

- Besides solution x_* also smoother solution $x_{*,p} = (A^*A)^{p/2}x_*$ with $y_* = Ax_{*,p}$, $p = 2$ was used.
- The problems were normalized, so that Euclidean norms of the operator and the right hand side were 1.
- For perturbed data we took $y = y_* + \Delta$, $\|\Delta\| = 0.3,\ 10^{-1},\ \ldots,\ 10^{-6}$ with 10 different normally distributed perturbations Δ generated by computer.
- Problems were solved by Tikhonov method, assuming that the noise level is $\delta = \varrho\|y - y_*\|$. Thus $\varrho > 1$ corresponds to overestimation of the true error, $\varrho < 1$ to underestimation.
- To compare the rules, we present averages (over problems, perturbations Δ and runs) of error ratios $\|x_\alpha - x_*\|/e_{\text{opt}}$, where e_{opt} is minimal error in Tikhonov method.

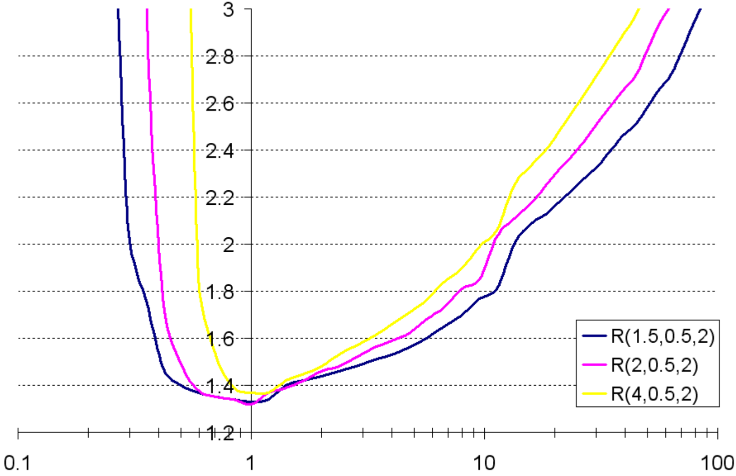
Stability of the rules with respect to $\varrho = \frac{\delta}{\|y-y_*\|}$



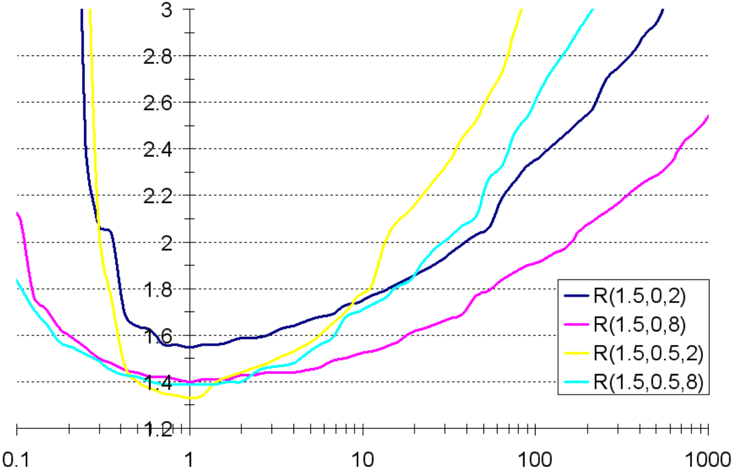
Stability of rule R(q, l, k) increases if k increases



Stability of rule R(q, l, k) increases if q decreases



$l = 0.5$ is recommended ($l = 0$ is good if $\delta \gg \|y - y_*\|$)



Post-estimation of regularization parameter in case $\|y - y_*\| \le \delta$

- $\alpha_{\mathrm{ME}} \ge \alpha_{\mathrm{opt}} := \operatorname{argmin}\{\|x_\alpha - x_*\|,\ \alpha \ge 0\}$, computations suggest $\alpha_{\mathrm{MEe}} = 0.4\alpha_{\mathrm{ME}}$, if $\|y - y_*\| = \delta$.
- More stable with respect to overestimation of noise level is the choice $\alpha_{\mathrm{Me}} = \min(\alpha_{\mathrm{MEe}}, 1.4\alpha_{\mathrm{R}(\frac{3}{2},\ \frac{1}{2},\ 2)})$, $b = 0.023$.

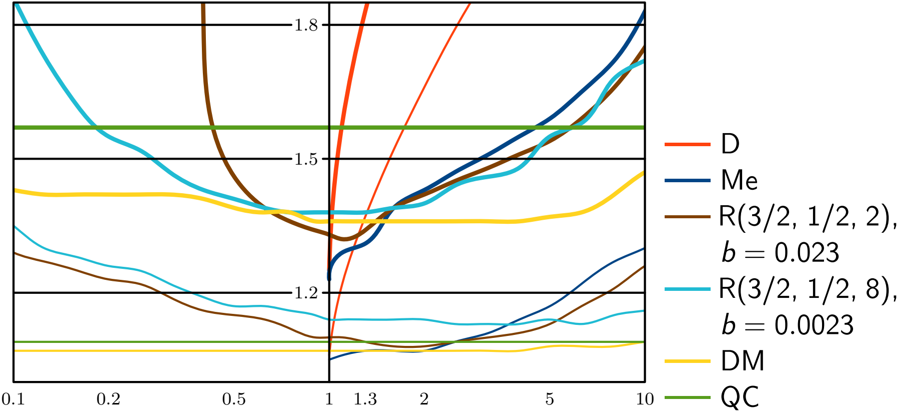
Heuristic rules (not using δ) in Tikhonov method

- **Quasioptimality criterion Q**: take α as the global minimizer of the function $\psi(\alpha) = \|x_\alpha - x_{2,\alpha}\|$, where $x_{2,\alpha}$ is 2-iterated Tikhonov approximation $x_{2,\alpha} = (\alpha I + A^*A)^{-1}(\alpha x_\alpha + A^*y)$. Sometimes this gives too small α, therefore we try to find a lower bound of minimization interval, determined during computations.
- **Rule QC**. Make computations on the sequence of parameters $\alpha_i = q^{i-1}$, $i = 1, 2, \ldots;$ $q < 1$, for example, $q = 0.9$. Take α_i as the minimizer of the function $\psi(\alpha_i) = \|x_{\alpha_i} - x_{2,\alpha_i}\|$ in the interval $[\underline{\alpha}, 1]$, where $\underline{\alpha}$ is the largest α_i, for which the value of $\psi(\alpha_i)$ is $C = 5$ times larger than its value at its current minimum.
- L-curve rule, GCV-rule, Hanke-Raus rule and Brezinski-Rodriguez-Seatzu rule gave in our numerical experiments not so good results as rules Q and QC.

Rule DM for approximate noise level in Tikhonov method

- **Rule DM for Tikhonov method**
  1) Make computations on the sequence of parameters $\alpha_i = q^{i-1}$, $i = 1, 2, \ldots$; $q < 1$, for example, $q = 0.9$; find $\underline{\alpha}$ as the first α_i for which $\sqrt{\alpha_i}\|x_{\alpha_i} - x_{2,\alpha_i}\| \leq c_1\delta$, $c_1 = \text{const}$;
  2) find $\alpha_i = \operatorname{argmin} \frac{(1+\alpha\|A\|^{-2})\|D_\alpha^{1/2}B_\alpha(Ax_\alpha - y)\|^2}{\alpha^{c_2}\|D_\alpha^{1/2}B_\alpha^2(Ax_\alpha - y)\|}$ in $[\underline{\alpha}, 1]$, $c_2 = \text{const}$.
- If $\varrho := \delta/\|y - y_*\| \in (0.1, 10)$, then we recommend $c_1 = 0.005$, $c_2 = 0.05$; if less information is known, $\varrho \in (0.01, 100)$, then we recommend $c_1 = 0.001$, $c_2 = 0.47$.
- Convergence $x_\alpha \to x_*$, as $\delta \to 0$, provided that $\lim \|y - y_*\|/\delta \leq C$, is guaranteed. If $x_* \in \mathcal{R}((A^*A)^{p/2})$, then for rule DM with $c_1 \geq 0.24$ the error estimate $\|x_\alpha - x_*\| \leq \text{const}\, \delta^{p/(p+1)}$ holds for all $p \leq 2$.

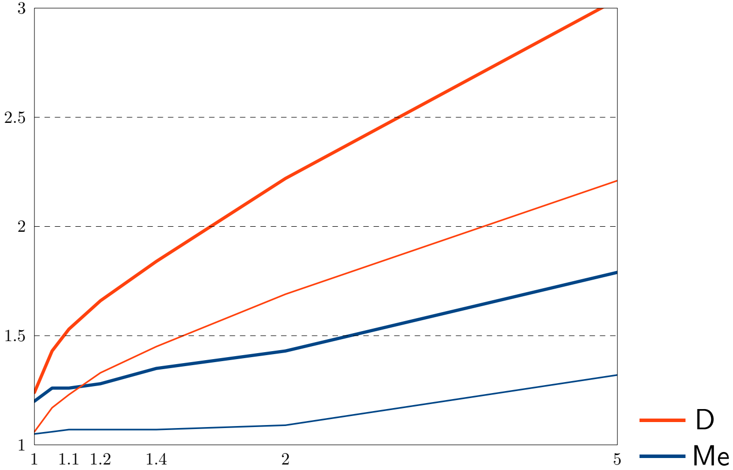
Averages (thick lines) and medians (thin lines) of error ratios in various rules in dependence of $\varrho = \delta / \|y - y_*\|$



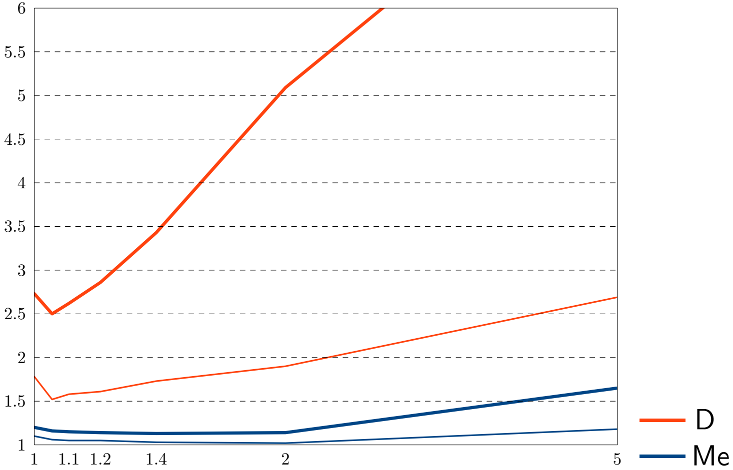
Preferences of rules in dependence of the accuracy of noise level information $\varrho = \delta / \|y - y_*\|$

- If we are sure that $\varrho \in [1, 1.5]$, then we recommend the rule Me.
- In case $\varrho \in [0.6, 1.5]$ we recommend the rule R(3/2, 1/2, 2), $b = 0.023$.
- If less information about the noise level is known, for example, $\varrho \in [1/20, 20]$, then we recommend the rule DM.
- For even less information about the noise level, we recommend the rule QC. If $\|Ax_{\alpha_{\mathrm{QC}}} - y\|$ is evidently less than $\|y - y_*\|$, then we recommend to decrease the constant C, for example, using $(C+1)/2$ instead of C.

Averages (thick lines) and medians (thin lines) of error ratios in rules D and Me in dependence of $\varrho = \delta / \|y - y_*\|$, $p = 0$



Averages (thick lines) and medians (thin lines) of error ratios in rules D and Me in dependence of $\varrho = \delta/\|y - y_*\|$, $p = 2$



Conclusions

- We propose a family of rules R(q, l, k) for approximate noise level, where $3/2 \le q < \infty$, $l \ge 0$, $k \ge l/q$, $2q, 2k, 2l \in \mathbb{N}$.
- If $k > l/q$ and $\frac{\|y - y_*\|}{\delta} \le C = \text{const}$ as $\delta \to 0$, then we have $\|x_\alpha - x_*\| \to 0$ $(\delta \to 0)$.
- Certain rules from the family gave in numerical experiments good results in case of several times over- or underestimated noise level.

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